

# On crystal ground state in the Schrödinger–Poisson model with point ions

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## Abstract

A space-periodic ground state is shown to exist for lattices of point ions in  $\mathbb{R}^3$  coupled to the Schrödinger and scalar fields. The coupling requires the renormalization due to the singularity of the Coulomb selfaction. The ground state is constructed by minimization of the renormalized energy per cell. This energy is bounded from below when the charge of each ion is positive. The elementary cell is necessarily neutral.

*Keywords:* crystal; lattice; ion; charge; wave function; potential; Schroedinger equation; Poisson equation; renormalization; elementary cell; energy per cell; Coulomb energy; minimization; neutrality condition; spectrum; embedding theorems; Fourier transform; infrared divergence; variation

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# 1 Introduction

We consider 3-dimensional crystal lattices in  $\mathbb{R}^3$ ,

$$(1.1) \quad \Gamma := \{\mathbf{x}(\mathbf{n}) = \mathbf{a}_1 n_1 + \mathbf{a}_2 n_2 + \mathbf{a}_3 n_3 : \mathbf{n} = (x_1, x_2, x_3) \in \mathbb{Z}^3\},$$

$\mathbf{a}_k \in \mathbb{R}^3$  are linearly independent periods. Born and Oppenheimer [6] developed the quantum dynamical approach to the crystal structure, separating the motion of ‘light electrons’ and of ‘heavy ions’. As an extreme form of this separation, the ions could be considered as classical nonrelativistic particles governed by the Lorentz equations neglecting the magnetic field, while the electrons could be described by the Schrödinger equation neglecting the electron spin. The scalar potential is the solution to the corresponding Poisson equation.

We consider the crystal with  $N$  ions per cell. Let  $\sigma_j(\mathbf{y}) = |e|Z_j\delta(\mathbf{y})$  be the charge density and  $M_j > 0$  the mass of the corresponding ion,  $j = 1, \dots, N$ . Then the coupled equations read

$$(1.2) \quad i\hbar\psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x}, t) + e\phi(\mathbf{x}, t)\psi(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^3,$$

$$(1.3) \quad \left[\frac{1}{c^2}\partial_t^2 - \Delta\right]\phi(\mathbf{x}, t) = \rho(\mathbf{x}, t) := \sum_{j=1}^N \sum_{\mathbf{n} \in \mathbb{Z}^3} \sigma_j(\mathbf{x} - \mathbf{x}(\mathbf{n}) - \mathbf{x}_j(\mathbf{n}, t)) + e|\psi(\mathbf{x}, t)|^2, \quad \mathbf{x} \in \mathbb{R}^3,$$

$$(1.4) \quad M_j\ddot{\mathbf{x}}_j(\mathbf{n}, t) = -|e|Z_j\nabla\phi_{\mathbf{n}, j}(\mathbf{x}(\mathbf{n}) + \mathbf{x}_j(\mathbf{n}, t)), \quad \mathbf{n} \in \mathbb{Z}^3, \quad j = 1, \dots, N.$$

Here  $e < 0$  is the electron charge,  $m$  is its mass,  $\psi(\mathbf{x}, t)$  denotes the wave function of the electron field, and  $\phi(\mathbf{x}, t)$  is the potential of the scalar field generated by the ions and the electrons. Further,  $(\cdot, \cdot)$  stands for the Hermitian scalar product in the Hilbert space  $L^2(\mathbb{R}^3)$ , and

$$(1.5) \quad \nabla\phi_{\mathbf{n}, j}(\mathbf{x}(\mathbf{n}) + \mathbf{x}_j(\mathbf{n}, t)) := \nabla_{\mathbf{y}} \left[ \phi(\mathbf{x}(\mathbf{n}) + \mathbf{x}_j(\mathbf{n}, t) + \mathbf{y}) - \frac{|e|Z_j}{4\pi|\mathbf{y}|} \right] \Big|_{\mathbf{y}=0}$$

All derivatives here and below are understood in the sense of distributions. The system is nonlinear and translation invariant, i.e.,  $\psi(\mathbf{x} - \mathbf{a}, t)$ ,  $\phi(\mathbf{x} - \mathbf{a}, t)$ ,  $\mathbf{x}_j(\mathbf{n}, t) + \mathbf{a}$  is also a solution for any  $\mathbf{a} \in \mathbb{R}^3$ .

A dynamical quantum description of the solid state as many-body system is not rigorously established yet (see Introduction of [26] and Preface of [30]). Up to date rigorous results concern only the ground state in different models (see below).

The classical ‘one-electron’ theory of Bethe-Sommerfeld, based on periodic Schrödinger equation, does not take into account oscillations of ions. Moreover, the choice of the periodic potential in this theory is very problematic, and corresponds to a fixation of the ion positions which are unknown.

The system (1.2)–(1.4) eliminates these difficulties though it does not respect the electron spin like the periodic Schrödinger equation. To remedy this deficiency we should replace the Schrödinger equation by the Hartree–Fock equations as the next step to more realistic model. However, we expect that the techniques developed for the system (1.2)–(1.4) will be useful also for more realistic dynamical models of crystals. These goals were our main motivation in writing this paper.

Here, we make the first step proving the existence of the ground state, which is a  $\Gamma$ -periodic stationary solution  $\psi^0(\mathbf{x})e^{-i\omega^0 t}$ ,  $\phi^0(\mathbf{x})$ ,  $\bar{\mathbf{x}} = (\mathbf{x}_1^0, \dots, \mathbf{x}_N^0)$  to the system (1.2)–(1.4):

$$(1.6) \quad \hbar\omega^0\psi^0(\mathbf{x}) = -\frac{\hbar^2}{2m}\Delta\psi^0(\mathbf{x}) + e\phi^0(\mathbf{x})\psi^0(\mathbf{x}), \quad \mathbf{x} \in T^3,$$

$$(1.7) \quad -\Delta\phi^0(\mathbf{x}) = \rho^0(\mathbf{x}) := \sigma^0(\mathbf{x}) + e|\psi^0(\mathbf{x})|^2, \quad \mathbf{x} \in T^3,$$

$$(1.8) \quad 0 = -|e|Z_j\nabla\phi_{\mathbf{n}, j}^0(\mathbf{x}_j^0), \quad j = 1, \dots, N.$$

Here,  $T^3 := \mathbb{R}^3/\Gamma$  denotes the ‘elementary cell’ of the crystal,  $\langle \cdot, \cdot \rangle$  stands for the Hermitian scalar product in the complex Hilbert space  $L^2(T^3)$  and its different extensions, and

$$(1.9) \quad \sigma^0(\mathbf{x}) := \sum_{j=1}^N \sigma_j(\mathbf{x} - \mathbf{x}_j^0), \quad \sigma_j(\mathbf{y}) := |e|Z_j\delta(\mathbf{y}).$$

The right hand side of (1.8) is defined similarly to (1.5):

$$(1.10) \quad \nabla \phi_{n,j}^0(\mathbf{x}_j^0) := \nabla_{\mathbf{y}} \left[ \phi(\mathbf{x}_j^0 + \mathbf{y}) - \frac{|e|Z_j}{4\pi|\mathbf{y}|} \right] \Big|_{\mathbf{y}=0}$$

The system (1.6)–(1.8) is translation invariant similarly to (1.2)–(1.4). Let us note that  $\omega^0$  should be real since  $\text{Im } \omega^0 \neq 0$  means an instability of the ground state: the decay as  $t \rightarrow \infty$  in the case  $\text{Im } \omega^0 < 0$  and the explosion if  $\text{Im } \omega^0 > 0$ . We have

$$(1.11) \quad \int_{T^3} \sigma^0(\mathbf{x}) d\mathbf{x} = Z|e|, \quad Z := \sum_j Z_j.$$

The total charge per cell should be zero (cf. [3]):

$$(1.12) \quad \int_{T^3} \rho^0(\mathbf{x}) d\mathbf{x} = \int_{T^3} [\sigma^0(\mathbf{x}) + e|\psi^0(\mathbf{x})|^2] d\mathbf{x} = 0.$$

This neutrality condition follows directly from equation (1.7) by integration using  $\Gamma$ -periodicity of  $\phi^0(\mathbf{x})$ . Equivalently, the neutrality condition can be written as the normalization

$$(1.13) \quad \int_{T^3} |\psi^0(\mathbf{x})|^2 d\mathbf{x} = Z.$$

Our main condition is the following:

$$(1.14) \quad \textbf{Positivity condition:} \quad Z_j > 0, \quad j = 1, \dots, N.$$

Let us comment on our approach. The neutrality condition (1.13) defines the submanifold  $\mathcal{M}$  in the space  $H^1(T^3) \times (T^3)^N$  of space-periodic configurations  $(\psi^0, \bar{\mathbf{x}}^0)$ . We construct a ground state as a minimizer over  $\mathcal{M}$  of the energy per cell (2.3). Previously we have established similar results [17] for the crystals with 1D, 2D and 3D lattices of smeared ions in  $\mathbb{R}^3$ . Our main novelties in the present paper are the following.

- I. We extend our results [17] to the point ions subtracting the infinite selfaction in the renormalized equations.
- II. We renormalize the energy per cell subtracting the infinite Coulomb selfaction of the point ions.
- III. We prove the bound from below for the renormalized energy under the novel assumption (1.14) of the positivity for the charge of each ion.

The minimization strategy ensures the existence of a ground state for any lattice (1.1). One could expect that a stable lattice should provide a local minimum of the energy per cell for fixed  $N$  and  $Z_j$ , but this is still an open problem.

Let us comment on related works. For atomic systems in  $\mathbb{R}^3$ , a ground state was constructed by Lieb, Simon and P. Lions in the case of the Hartree and Hartree–Fock models [25, 27, 28], and by Nier for the Schrödinger–Poisson model [29]. The Hartree–Fock dynamics for molecular systems in  $\mathbb{R}^3$  has been constructed by Cancès and Le Bris [7].

A mathematical theory of the stability of matter started from the pioneering works of Dyson, Lebowitz, Lenard, Lieb and others for the Schrödinger many body model [14, 21, 22, 24]; see the survey in [18]. Recently, the theory was extended to the quantized Maxwell field [23].

These results and methods were developed last two decades by Blanc, Le Bris, Catto, P. Lions and others to justify the thermodynamic limit for the Thomas–Fermi and Hartree–Fock models with space-periodic ion arrangement [4, 10, 11, 12] and to construct the corresponding space-periodic ground states [13], see the survey and further references in [5].

Recently, Giuliani, Lebowitz and Lieb have established the periodicity of the thermodynamic limit in 1D local mean field model without the assumption of periodicity of the ion arrangement [15].

Cancès and others studied short-range perturbations of the Hartree–Fock model and proved that the density matrices of the perturbed and unperturbed ground states differ by a compact operator, [8, 9].

The Hartree–Fock dynamics for infinite particle systems were considered recently by Cancès and Stoltz [9], and Lewin and Sabin [19]. In [9], the well-posedness is established for local perturbations of the periodic ground state density matrix in an infinite crystal. However, the space-periodic nuclear potential in the equation [9, (3)] is fixed that corresponds to the fixed nuclei positions. Thus the back reaction of the electrons onto the nuclei is neglected. In [19], the well-posedness is established for the von Neumann equation with density matrices of infinite trace for pair-wise interaction potentials  $w \in L^1(\mathbb{R}^3)$ . Moreover, the authors prove the asymptotic stability of the ground state in 2D case [20]. Nevertheless, the case of the Coulomb potential for infinite particle systems remains open since the corresponding generator is infinite.

The plan of our paper is as follows. In Section 2, we renormalize the energy per cell and prove that the renormalized energy is bounded from below. In Section 3, we prove the compactness of the minimizing sequence, and in Section 4 calculate the energy variation. In the final Section 5, we prove the Schrödinger equation.

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## 2 The renormalized energy per cell

We consider the system (1.6), (1.7) for the corresponding functions on the torus  $T^3 = \mathbb{R}^3/\Gamma$  and for  $\mathbf{x}_{0j} \bmod \Gamma \in T^3$ . For  $s \in \mathbb{R}$ , we denote by  $H^s$  the Sobolev space on the torus  $T^3$ , and for  $1 \leq p \leq \infty$ , we denote by  $L^p$  the Lebesgue space of functions on  $T^3$ .

The ground state will be constructed by minimizing the energy in the cell  $T^3$ . To this aim, we will minimize the energy with respect to  $\bar{\mathbf{x}} := (\mathbf{x}_1, \dots, \mathbf{x}_N) \in (T^3)^N$  and  $\psi \in H^1$  satisfying the neutrality condition (1.12):

$$(2.1) \quad \int_{T^3} \rho(\mathbf{x}) d\mathbf{x} = 0, \quad \rho(\mathbf{x}) := \sigma(\mathbf{x}) + v(\mathbf{x}),$$

where we set

$$(2.2) \quad \sigma(\mathbf{x}) := \sum_j \sigma_j(\mathbf{x} - \mathbf{x}_j), \quad v(\mathbf{x}) := e|\psi(\mathbf{x})|^2$$

similarly to (1.9). Let us note that the charge densities  $\sigma$  and  $\rho$  are finite Borelian measures on  $T^3$  for  $\psi \in H^1$  since  $\psi \in L^6$  by the Sobolev embedding theorem.

For sufficiently smooth (smeared) ion densities  $\sigma(\mathbf{x})$  the energy in the periodic cell is defined as in [17]:

$$(2.3) \quad E(\psi, \bar{\mathbf{x}}) := \frac{\hbar^2}{2m} \langle \nabla \psi(\mathbf{x}), \nabla \psi(\mathbf{x}) \rangle + \frac{1}{2} \langle \phi, \rho \rangle, \quad \phi := Q\rho$$

where  $\langle \cdot, \cdot \rangle$  denotes the Hermitian scalar product in  $L^2$ , and  $Q\rho := (-\Delta)^{-1}\rho$  is well-defined by (2.1). Namely, consider the dual lattice

$$(2.4) \quad \Gamma^* = \{\mathbf{k}(\mathbf{n}) = \mathbf{b}_1 n_1 + \mathbf{b}_2 n_2 + \mathbf{b}_3 n_3 : \mathbf{n} = (n_1, n_2, n_3) \in \mathbb{Z}^3\},$$

where  $\mathbf{b}_k \mathbf{a}_{k'} = 2\pi \delta_{kk'}$ . Every finite measure  $\rho$  on  $T^3$  admits the Fourier representation

$$(2.5) \quad \rho(\mathbf{x}) = \frac{1}{\sqrt{|T^3|}} \sum_{\mathbf{k} \in \Gamma^*} \hat{\rho}(\mathbf{k}) e^{-i\mathbf{k}\mathbf{x}}, \quad \hat{\rho}(\mathbf{k}) = \frac{1}{\sqrt{|T^3|}} \int_{T^3} e^{i\mathbf{k}\mathbf{x}} \rho(\mathbf{x}) d\mathbf{x}.$$

where the Fourier coefficients  $\hat{\rho}(\mathbf{k})$  are bounded. Respectively, we define the Coulomb potential

$$(2.6) \quad \phi(\mathbf{x}) = Q\rho(\mathbf{x}) := \frac{1}{\sqrt{|T^3|}} \sum_{\mathbf{k} \in \Gamma^* \setminus 0} \frac{\hat{\rho}(\mathbf{k})}{\mathbf{k}^2} e^{-i\mathbf{k}\mathbf{x}}.$$

This function  $\phi \in L^2$  and satisfies the Poisson equation  $-\Delta\phi = \rho$ , since  $\hat{\rho}(0) = 0$  due to the neutrality condition (2.1). Finally,

$$(2.7) \quad \int_{T^3} \phi(\mathbf{x}) d\mathbf{x} = 0.$$

For the smeared ions the energy (2.3) can be rewritten as

$$(2.8) \quad E(\psi, \bar{\mathbf{x}}) = \frac{\hbar^2}{2m} \langle \nabla \psi, \nabla \psi \rangle + \frac{1}{2} \langle Q\sigma, \sigma \rangle + \langle Q\sigma, v \rangle + \frac{1}{2} \langle Qv, v \rangle.$$

Let us show that for the point ions the Coulomb selfaction energy  $\langle Q\sigma, \sigma \rangle = \sum_{j,k=1}^N \langle Q\sigma_j, \sigma_k \rangle$  is infinite. Namely, according to (2.6), the Coulomb potential of the ions reads

$$(2.9) \quad \phi_{\text{ions}}(\mathbf{x}) := Q\sigma(\mathbf{x}) = \frac{1}{\sqrt{|T^3|}} \sum_{\mathbf{k} \in \Gamma^* \setminus 0} \frac{\hat{\sigma}(\mathbf{k})}{\mathbf{k}^2}, \quad \hat{\sigma}(\mathbf{k}) = \frac{|e|}{\sqrt{|T^3|}} \sum_j Z_j e^{i\mathbf{k}\mathbf{x}_j}.$$

Hence, for the point ions

$$(2.10) \quad \phi_{\text{ions}}(\mathbf{x}) = \sum_j \phi_j(\mathbf{x}), \quad \phi_j(\mathbf{x}) := Q\sigma_j(\mathbf{x} - \mathbf{x}_j) = |e| Z_j G(\mathbf{x} - \mathbf{x}_j), \quad G(\mathbf{x}) = \sum_{\mathbf{k} \in \Gamma^* \setminus 0} \frac{e^{-i\mathbf{k}\mathbf{x}}}{\mathbf{k}^2}$$

where  $G(\mathbf{x})$  is the Green function introduced in [11]. Obviously,  $\int_{T^3} G(\mathbf{x}) d\mathbf{x} = 0$ , and  $-\Delta G(\mathbf{x}) = \delta(\mathbf{x})$ . Therefore, by the elliptic regularity,

$$(2.11) \quad G \in C^\infty(T^3 \setminus 0), \quad D(\mathbf{x}) := G(\mathbf{x}) - \frac{1}{4\pi|\mathbf{x}|} \in C^\infty(|\mathbf{x}| < \varepsilon)$$

for sufficiently small  $\varepsilon > 0$ . As the result, the selfaction terms  $\langle Q\sigma_j(\mathbf{x} - \mathbf{x}_j), \sigma_j(\mathbf{x} - \mathbf{x}_j) \rangle = |e|^2 Z_j^2 G(0)$  are infinite, while  $\langle Q\sigma_j(\mathbf{x} - \mathbf{x}_j), \sigma_k(\mathbf{x} - \mathbf{x}_k) \rangle = |e|^2 Z_j Z_k G(\mathbf{x}_j - \mathbf{x}_k)$  are finite for  $j \neq k$ .

**Remark 2.1.** Let us note that  $G(\mathbf{x})$  is symmetric with respect to the reflection  $\mathbf{x} \mapsto -\mathbf{x}$  of the torus  $T^3$ . Therefore, the difference  $D(\mathbf{x})$  is symmetric in the ball  $|\mathbf{x}| < \varepsilon$  with respect to this reflection, and hence

$$(2.12) \quad \nabla D(0) = 0.$$

From now on we consider the point ions (1.9), and we will renormalize the energy (2.8) subtracting the infinite selfaction terms:

$$(2.13) \quad E_r(\psi, \bar{\mathbf{x}}) = \frac{\hbar^2}{2m} \langle \nabla \psi, \nabla \psi \rangle + \frac{1}{2} \sum_{j \neq k} \langle Q\sigma_j(\mathbf{x} - \mathbf{x}_j), \sigma_k(\mathbf{x} - \mathbf{x}_k) \rangle + \langle Q\sigma, v \rangle + \frac{1}{2} \langle Qv, v \rangle.$$

Let us note that  $v \in L^2$  for  $\psi \in H^1$  by the Sobolev embedding theorem, and  $Q\sigma \in L^2$ . Hence, the renormalized energy is finite for  $\psi \in H^1$ . Next problem is to check that the renormalized energy is bounded from below. Let us denote

$$(2.14) \quad \mathcal{X} := \{\bar{\mathbf{x}} \in (T^3)^N : \mathbf{x}_j \neq \mathbf{x}_k \text{ for } j \neq k\}, \quad d(\bar{\mathbf{x}}) := \min_{j \neq k} \text{dist}(\mathbf{x}_j, \mathbf{x}_k).$$

**Definition 2.2.**  $\mathcal{M} := M \times \mathcal{X}$ , where  $M$  denotes the manifold (cf. (1.13))

$$(2.15) \quad M = \{\psi \in H^1 : \int_{T^3} |\psi(\mathbf{x})|^2 d\mathbf{x} = Z\}$$

endowed with the topology of  $H^1 \times \mathcal{X}$ .

**Lemma 2.3.** Let condition (1.14) hold. Then the functional  $E_r$  is continuous on  $\mathcal{M}$ , and the bound holds

$$(2.16) \quad E_r(\psi, \bar{\mathbf{x}}) \geq \varepsilon \|\psi\|_{H^1}^2 + \frac{q}{d(\bar{\mathbf{x}})} + \frac{1}{2} \langle Q\psi, \psi \rangle - C, \quad (\psi, \bar{\mathbf{x}}) \in \mathcal{M},$$

where  $q, \varepsilon > 0$ .

**Proof.** First,  $v := e|\psi(\mathbf{x})|^2 \in L^2$  since  $\|v\|_{L^2} = e^2 \|\psi\|_{L^4}^2 \leq C_1 \|\psi\|_{H^1}^2$  by the Sobolev embedding theorem [1, 31]. Further,  $Q\sigma \in L^2$  since  $\sigma$  is the finite Borelian measure on  $T^3$  by (2.2). Hence, for any  $\delta > 0$

$$(2.17) \quad |\langle Q\sigma(\mathbf{x}), v(\mathbf{x}) \rangle| \leq C \|\psi\|_{L^4}^2 \leq \delta \|\psi\|_{L^6}^2 + C(\delta) \|\psi\|_{L^2}^2 \leq C_2 \delta \|\psi\|_{H^1}^2 + C(\delta)Z.$$

Here the second inequality follows by the Young inequality from  $\|\psi\|_{L^4} \leq \|\psi\|_{L^6}^{3/4} \|\psi\|_{L^2}^{1/4}$  which holds by the Riesz convexity theorem. This theorem follows by the Hölder inequality, and in our case the Cauchy-Schwarz is sufficient:

$$\int |\psi(\mathbf{x})|^3 |\psi(\mathbf{x})| d\mathbf{x} \leq \left[ \int |\psi(\mathbf{x})|^6 d\mathbf{x} \right]^{1/2} \left[ \int |\psi(\mathbf{x})|^2 d\mathbf{x} \right]^{1/2}.$$

Therefore, the functional  $(\psi, \bar{\mathbf{x}}) \mapsto \langle Q\sigma, v \rangle$  is continuous on  $\mathcal{M}$  in the topology of  $H^1 \times \mathcal{X}$ .

On the other hand, for  $\psi \in M$  we have  $\|\psi\|_{H^1}^2 = \int_{T^3} |\nabla \psi(\mathbf{x})|^2 d\mathbf{x} + Z$ . Hence, the bound (2.16) follows if we take  $C_2 \delta < \frac{h^2}{2m}$ . ■

### 3 Compactness of minimizing sequence

The energy is finite and bounded from below on the manifold  $\mathcal{M}$  by Lemma 2.3. Hence, there exists a minimizing sequence  $(\psi_n, \bar{\mathbf{x}}_n) \in \mathcal{M}$  such that

$$(3.1) \quad E_r(\psi_n, \bar{\mathbf{x}}_n) \rightarrow E_r^0 := \inf_{\mathcal{M}} E(\psi, \bar{\mathbf{x}}), \quad n \rightarrow \infty.$$

**Remark 3.1.** For sufficiently smooth charge densities  $\sigma_j$  the energy (2.8) is also finite, and its difference with (2.13) equals  $\frac{1}{2} \sum \langle Q\sigma_j(\mathbf{x} - \mathbf{x}_j), \sigma_j(\mathbf{x} - \mathbf{x}_j) \rangle = \frac{1}{2} \sum \langle Q\sigma_j, \sigma_j \rangle$ . This difference does not depend on  $\psi$  and  $\bar{\mathbf{x}}$ . Hence, the corresponding minimizers coincide.

Our main result is the following:

**Theorem 3.2.** i) There exists  $(\psi^0, \bar{\mathbf{x}}^0) \in \mathcal{M}$  with

$$(3.2) \quad E_r(\psi^0, \bar{\mathbf{x}}^0) = E_r^0.$$

ii) Moreover,  $\psi^0$  satisfies equations (1.6)–(1.8) with a real potential  $\phi^0 \in L^2$  and  $\omega^0 \in \mathbb{R}$ .

To prove i), let us denote

$$(3.3) \quad \rho_n(\mathbf{x}) := \sigma_n(\mathbf{x}) + e|\psi_n(\mathbf{x})|^2, \quad \sigma_n(\mathbf{x}) := \sum_j \mu_j^{\text{per}}(\mathbf{x} - \mathbf{x}_{jn}), \quad v_n(\mathbf{x}) := e|\psi_n(\mathbf{x})|^2.$$

The sequence  $\psi_n$  is bounded in  $H^1$  by (3.1) and (2.16), and hence the corresponding sequence  $v_n$  is bounded in  $L^2$  by the Sobolev embedding theorem [1, 31]. Respectively, the corresponding sequences  $Q\sigma_n$  and  $\phi_n := Q\rho_n$  are bounded in  $L^2$ .

Hence, the sequence  $\psi_n$  is precompact in  $L^p$  for any  $p \in [1, 6)$  by the Sobolev embedding theorem. As the result, there exist a subsequence  $n' \rightarrow \infty$  for which

$$(3.4) \quad \psi_{n'} \xrightarrow{L^p} \psi^0, \quad v_{n'}(\mathbf{x}) \xrightarrow{L^2} v^0, \quad \phi_{n'} \xrightarrow{L_w^2} \phi^0, \quad \bar{\mathbf{x}}_{n'} \rightarrow \bar{\mathbf{x}}^0 \in \mathcal{X}, \quad n' \rightarrow \infty$$

with any  $p \in [1, 6)$ . Respectively, the convergences

$$(3.5) \quad \sigma_{n'} \rightarrow \sigma^0, \quad \rho_{n'} \rightarrow \rho^0, \quad n' \rightarrow \infty.$$

hold in the sense of distributions, where  $\sigma^0(\mathbf{x})$  and  $\rho^0(\mathbf{x})$  are defined by (1.9) and (1.7). Therefore,

$$(3.6) \quad Q\sigma_{n'} \xrightarrow{L_w^2} Q\sigma^0, \quad n' \rightarrow \infty.$$

Hence, the neutrality condition (1.12) holds,  $(\psi^0, \bar{\mathbf{x}}^0) \in \mathcal{M}$ ,  $\phi^0 \in L^2$ , and for these limit functions we have

$$(3.7) \quad -\Delta\phi^0 = \rho^0, \quad \int_{T^3} \phi^0(\mathbf{x}) d\mathbf{x} = 0.$$

To prove identity (3.2), we write the energy (2.13) as the sum  $E_r = E_1 + E_2 + E_3 + E_4$ , where

$$\begin{aligned} E_1(\psi, \bar{\mathbf{x}}) &= \frac{\hbar^2}{2m} \langle \nabla \psi(\mathbf{x}), \nabla \psi(\mathbf{x}) \rangle, & E_2(\psi, \bar{\mathbf{x}}) &= \frac{1}{2} \sum_{j \neq k} \langle Q\sigma(\mathbf{x} - \mathbf{x}_j), \sigma(\mathbf{x} - \mathbf{x}_k) \rangle, \\ E_3(\psi, \bar{\mathbf{x}}) &= \langle Q\sigma(\mathbf{x}), v(\mathbf{x}) \rangle, & E_4(\psi, \bar{\mathbf{x}}) &= \frac{1}{2} \langle Qv(\mathbf{x}), v(\mathbf{x}) \rangle. \end{aligned}$$

Finally, the convergences (3.4) and (3.6) imply that

$$E_1(\psi^0, \bar{\mathbf{x}}^0) \leq \liminf_{n' \rightarrow \infty} E_1(\psi_{n'}, \bar{\mathbf{x}}_{n'}), \quad E_l(\psi^0, \bar{\mathbf{x}}^0) = \lim_{n' \rightarrow \infty} E_l(\psi_{n'}, \bar{\mathbf{x}}_{n'}), \quad l = 2, 3, 4.$$

These limits, together with (3.1), give that  $E_r(\psi^0, \bar{\mathbf{x}}^0) \leq E_r^0$ . Now (3.2) follows from the definition of  $E_r^0$ , since  $(\psi^0, \bar{\mathbf{x}}^0) \in \mathcal{M}$ . Thus Theorem 3.2 i) is proved.

We will prove Theorem 3.2 ii) in next sections.

## 4 Variation of the energy

Theorem 3.2 ii) follows from next proposition.

**Proposition 4.1.** *The limit functions (3.4) satisfy equations (1.6)–(1.8) with  $\omega^0 \in \mathbb{R}$ .*

The Poisson equation (1.7) is proved in (3.7). The Lorentz equation (1.8) follows by differentiation of the energy (2.13) in  $\mathbf{x}_j$ . Namely, the derivative at the minimal point  $(\psi^0, \bar{\mathbf{x}}^0)$  should vanish: taking into account (2.10), we obtain

$$\begin{aligned} 0 &= \nabla_{\mathbf{x}_j} E_r(\psi^0, \bar{\mathbf{x}}^0) = \sum_{k \neq j} \langle Q\nabla \sigma_j(\mathbf{x} - \mathbf{x}_j^0), \sigma_k(\mathbf{x} - \mathbf{x}_k^0) \rangle + \langle Q\nabla \sigma_j(\mathbf{x} - \mathbf{x}_j^0), v^0 \rangle \\ &= \langle \nabla \sigma_j(\mathbf{x} - \mathbf{x}_j^0), \phi^0(\mathbf{x}) - \phi_j^0(\mathbf{x}) \rangle = -\langle \sigma_j(\mathbf{x} - \mathbf{x}_j^0), \nabla[\phi^0(\mathbf{x}) - \phi_j^0(\mathbf{x})] \rangle, \end{aligned}$$

where  $\phi_j^0(\mathbf{x}) := Q\sigma_j(\mathbf{x} - \mathbf{x}_j^0)$  similarly to (2.10). Finally, the last expression coincides with the right hand side of (1.8) by its definition (1.10) together with (2.12).

It remains to prove the Schrödinger equation (1.6). Let us denote  $\mathcal{E}_r(\psi) := E_r(\psi, \bar{\mathbf{x}}^0)$ . We derive (1.6) in next sections, equating the variation of  $\mathcal{E}_r(\cdot)|_M$  to zero at  $\psi = \psi^0$ . In this section we calculate the corresponding Gâteaux variational derivative.

We should work directly on  $M$  introducing an atlas in a neighborhood of  $\psi^0$  in  $M$ . We define the atlas as the stereographic projection from the tangent plane  $TM(\psi^0) = (\psi^0)^\perp := \{\psi \in H^1 : \langle \psi, \psi^0 \rangle = 0\}$  to the sphere (2.15):

$$(4.1) \quad \psi_\tau = \frac{\psi^0 + \tau}{\|\psi^0 + \tau\|_{L^2}} \sqrt{Z}, \quad \tau \in (\psi^0)^\perp.$$

Obviously,

$$(4.2) \quad \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \psi_{\varepsilon\tau} = \tau, \quad \tau \in (\psi^0)^\perp,$$

where the derivative exists in  $H^1$ . We define the 'Gâteaux derivative' of  $\mathcal{E}_r(\cdot)|_M$  as

$$(4.3) \quad D_\tau \mathcal{E}_r(\psi^0) := \lim_{\varepsilon \rightarrow 0} \frac{\mathcal{E}_r(\psi_{\varepsilon\tau}) - \mathcal{E}_r(\psi^0)}{\varepsilon},$$

if this limit exists. We should restrict the set of allowed tangent vectors  $\tau$ .

**Definition 4.2.**  $\mathcal{T}^0$  is the space of test functions  $\tau \in (\psi^0)^\perp \cap C^\infty(T^3)$ .

Obviously,  $\mathcal{T}^0$  is dense in  $(\psi^0)^\perp$  in the norm of  $H^1$ .

**Lemma 4.3.** Let  $\tau \in \mathcal{T}^0$ . Then the derivative (4.3) exists, and

$$(4.4) \quad D_\tau \mathcal{E}_r(\psi^0) = \int_{T^3} \left[ \frac{\hbar^2}{2m} (\nabla \tau \overline{\nabla \psi^0} + \nabla \psi^0 \overline{\nabla \tau}) + e Q \rho^0 (\tau \overline{\psi^0} + \psi^0 \overline{\tau}) \right] d\mathbf{x}.$$

**Proof.** Let us denote  $v_{\varepsilon\tau}(\mathbf{x}) := e |\psi_{\varepsilon\tau}(\mathbf{x})|^2$ .

**Lemma 4.4.** For  $\tau \in \mathcal{T}^0$  we have  $v_{\varepsilon\tau} \in L^2$ , and

$$(4.5) \quad D_\tau v := \lim_{\varepsilon \rightarrow 0} \frac{v_{\varepsilon\tau} - v_0}{\varepsilon} = e (\tau \overline{\psi^0} + \psi^0 \overline{\tau}),$$

where the limit converges in  $L^2$ .

**Proof.** In the polar coordinates

$$(4.6) \quad \psi_{\varepsilon\tau} = (\psi^0 + \varepsilon \tau) \cos \alpha, \quad \alpha = \alpha(\varepsilon) = \arctan \frac{\varepsilon \|\tau\|_{L^2}}{\|\psi^0\|_{L^2}}.$$

Hence,

$$(4.7) \quad \begin{aligned} v_{\varepsilon\tau} &= e \cos^2 \alpha |\psi^0 + \varepsilon \tau|^2 \\ &= v^0 + e \varepsilon \cos^2 \alpha (\tau \overline{\psi^0} + \psi^0 \overline{\tau}) + e [\varepsilon^2 |\tau|^2 \cos^2 \alpha - |\psi^0|^2 \sin^2 \alpha]. \end{aligned}$$

It remains to estimate the last term of (4.7),

$$(4.8) \quad R_\varepsilon := \Lambda [\varepsilon^2 |\tau|^2 \cos^2 \alpha - |\psi^0|^2 \sin^2 \alpha].$$

Here  $|\psi^0|^2 \in L^2$  since  $\psi^0 \in H^1 \subset L^6$ . Finally,  $|\tau|^2 \in L^2$  and  $\sin^2 \alpha \sim \varepsilon^2$ . Hence, the convergence (4.5) holds in  $L^2$ . ■

Now (4.4) follows by differentiation in  $\varepsilon$  of (2.13) with  $\psi = \psi_{\varepsilon\tau}$ ,  $\sigma = \sigma^0$  and  $v = v_{\varepsilon\tau}$ . ■



## 5 The Schrödinger equation

Since  $\psi^0$  is a minimal point, the Gâteaux derivative (4.4) vanishes:

$$(5.1) \quad \int_{T_2} \left[ \frac{\hbar^2}{2m} (\nabla \tau \overline{\nabla \psi^0} + \nabla \psi^0 \overline{\nabla \tau}) + e Q \rho^0 (\tau \overline{\psi^0} + \psi^0 \overline{\tau}) \right] d\mathbf{x} = 0.$$

Substituting  $i\tau$  instead of  $\tau$  in this identity and subtracting, we obtain

$$(5.2) \quad -\frac{\hbar^2}{2m} \langle \Delta \psi^0, \tau \rangle + e \langle Q \rho^0, \overline{\psi^0} \tau \rangle = 0.$$

Finally,

$$(5.3) \quad \langle Q \rho^0, \overline{\psi^0} \tau \rangle = \langle \phi^0 \psi^0, \tau \rangle$$

since  $\rho^0 = -\Delta \phi^0$ . Hence, we can rewrite (5.2) as the variational identity

$$(5.4) \quad \left\langle -\frac{\hbar^2}{2m} \Delta \psi^0 + e \phi^0 \psi^0, \tau \right\rangle = 0, \quad \tau \in \mathcal{T}^0.$$

Now we can prove the Schrödinger equation (1.6).

**Lemma 5.1.**  $\psi^0$  is the eigenfunction of the Schrödinger operator  $H = -\frac{\hbar^2}{2m} \Delta + e \phi^0$ :

$$(5.5) \quad H \psi^0 = \lambda \psi^0,$$

where  $\lambda \in \mathbb{R}$ .

**Proof.** First,  $H \psi^0$  is a well-defined distribution since  $\phi^0, \psi^0 \in L^2$  by (3.4), and hence  $\phi^0 \psi^0 \in L^1$ . Second,  $\psi^0 \neq 0$  since  $\psi^0 \in M$  and  $Z > 0$ . Hence, there exists a test function  $\theta \in C^\infty(T^3) \setminus \mathcal{T}^0$ , i.e.,

$$(5.6) \quad \langle \psi^0, \theta \rangle \neq 0.$$

Then

$$(5.7) \quad \langle (H - \lambda) \psi^0, \theta \rangle = 0.$$

for an appropriate  $\lambda \in \mathbb{C}$ . However,  $(H - \lambda) \psi^0$  also annihilates  $\mathcal{T}^0$  by (5.4), hence it annihilates the whole space  $C^\infty(T^3)$ . This implies (5.5) in the sense of distributions with a  $\lambda \in \mathbb{C}$ . Finally, (5.5) gives

$$(5.8) \quad \langle H \psi^0, \psi^0 \rangle = \lambda \langle \psi^0, \psi^0 \rangle,$$

where the left hand side is well defined since  $\psi^0 \in H^1$  and  $\psi^0 \in L^4$ , while  $\phi^0 \in L^2$ . Therefore,  $\lambda \in \mathbb{R}$  since the potential is real. ■

This lemma implies equation (1.6) with  $\hbar \omega^0 = \lambda$ , and hence Theorem 3.2 ii) is proved.

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